CLAIMS

What is claimed is:

1. A method for identifying a potential inhibitor for a paramyxovirus Hemagglutinin-neuraminidase, comprising the steps of:

a, using a three-dimensional structure of the paramyxovirus hemagglutinen-neuraminidase as defined by the structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID NO: 1;

b. applying the three-dimensional structure to design or select the potential inhibitor;

c. obtaining the potential inhibitor;

d. associating the potential inhibitor with the enzyme in the presence of a substrate to determine the ability of the potential inhibitor to inhibit the enzyme.

2. The method according to claim 1, wherein the potential inhibitor is designed de novo.

3. The method according to claim 1, wherein the potential inhibitor is designed from a known inhibitor.

4. The method according to claim 1, wherein the step of employing the three-dimensional structure to design or select the compound comprises the steps of:

a. identifying chemical entities or fragments capable of associating with the enzyme; and

b. assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.

1   5. The method of according to claim 4, wherein the potential inhibitor is designed de

2   novo.

1   6. The method according to claim 4, wherein the potential inhibitor is designed from a

2   known inhibitor.

1   7. A complex of a paramyxovirus Hemagglutinin-neuraminidase and a substrate or

2   inhibitor molecule.

1   8.   The complex of claim 7 being obtained by diffusion or co-crystallization.

1   9. The method according to claim 1 wherein the potential inhibitor is a competitive,

2   noncompetitive , or uncompetitive inhibitor of a paramyoxvirus Hemagglutinin-

3   Neuraminidase.

1   10. The method according to claim 1 wherein the potential inhibitor is designed to form

2   salt links with Arg416 and Arg498 of a paramyxovirus hemagglutininneuraminidase.

1   11. The method according to claim 1 wherein the potential inhibitor is designed to form

2   hydrogen bonds or salt links with Glu258 of a paramyxovirus hemagglutinin-

3   neuraminidase.

1   12. The method according to claim 1 wherein the potential inhibitor is designed to form

2   hydrogen bonds or salt links with Lys 199 of a paramyxovirus hemagglutinin-

3   neuraminidase.

1   13.   The method of claim 1 which comprises using a three-dimensional structure of

2   paramyxovirus hemagglutnin-neuraminidase.

14.   The method of claim 13 wherein the paramyxovirus hemagglutnin-neuraminidase is Neucastle Disease Virus hemagglutnin neuraminidase.

15.   A machine readable data storage medium comprising a data storage material encoded with machine-readable data which comprises the structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID NO: 1.

16.   The machine-readable data storage medium of claim 15 wherein the machine-readable data comprises the three-dimensional structure of paramyxovirus Hemagglutnin-neuraminidase.

17.   The machine-readable data storage medium of claim 16 wherein the paramyxovirus Hemagglutnin-neuraminidase is Newcastle Disease Virus Hemagglutnin-Neuraminidase.

18.   A computer for producing a three-dimensional representation of:

        a.   a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID NO: 1; wherein the computer comprises:

                (i) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, comprising the structure coordinates comprising the amino acid residues 174, 175, 190, 192, 199, 234, 236, 237, 254, 256, 258, 262, 299, 302, 317, 363, 364, 369, 401, 416, 466, 498 and 526 according to SEQ ID

11 : 1;

12 (ii) a working memory for storing instructions for processing the machine-
13 readable data;

14 (iii) a central-processing unit coupled to the working memory and to the
15 machine-readable data storage medium for processing the machine readable data into the
16 three-dimensional representation; and

17 (iv) a display coupled to the central-processing unit for displaying the
18 three-dimensional representation.

1 19. The computer of claim 18 wherein the computer produces a three-dimensional representation of a paramyxovirus Hemagglutnin-neuraminidase; and

wherein the machine-readable data comprises the structure coordinates of paramyxovirus Hemagglutnin-neuraminidase.

20. The computer of claim 18 wherein the computer produces a three-dimensional representation of Newcastle Disease Virus Hemagglutnin Neuraminidase and wherein the machine readable data comprises the structure coordinates of Newcastle Disease Virus Hemagglutnin Neuraminidase.

1 21. The method of claim 1 which comprises:

2 employing computational means to perform a fitting operation between the
3 potential inhibitor and the structure coordinates of the three-dimensional structure; and

4 analyzing the results of the fitting operation to quantify the association between
5 the potential inhibitor and the structure coordinates.